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Discovery of a first-in-class topically bioavailable kit inhibitor with clinical activity using computational chemogenomics technology

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Abstract

Methods of computational chemogenomics have been used to discover kinase inhibitory activity in a number of clinically safe non-oncology drugs not previously known to inhibit any kinase or to interact with any nucleotide binding proteins. One of these drugs, NPH29, previously in development as a topical dual COX-2 / 5-LO inhibitor, was found to also inhibit Kit kinase with similar potency. Differing from systemically used Kit inhibitor oncology drugs, NPH29 has low molecular weight (MW < 300 Da) and other phys. chem. properties suitable for its topical use. Therapeutic relevance of the newly discovered activity of NPH29 against Kit was confirmed in a pilot clinical study - providing the first example of clinical validation of computationally predicted molecular activity leading to new therapeutic indications ("drug retargeting"). The discovery of a topically bioavailable Kit inhibitor NPH29 and rapid clinical confirmation of its activity illustrates the potential of systematic drug retargeting as a productive drug discovery strategy to address new therapeutic targets using existing investigational or approved drugs.

Biography

James Hendrix completed his Ph.D. and postdoctoral studies from Colorado State University in organic synthesis. He has over 20 years of experience in drug discovery working for Sanofi-Aventis and predecessor companies where he rose to the level of senior director of CNS Medicinal Chemistry. Currently he is the President of Technology at nPharmakon. He has track record of success in the discovery of drug candidates and lead chemical series. He published more than 30 patents and papers in reputable journals. He is also a member of several scientific advisory boards for both private companies and non-profit foundations.